Center for Materials Science of Nuclear Fuel
Interim EFRC Director: Todd Allen
Lead Institution: Idaho National Laboratory

***Mission Statement*:** to develop an experimentally validated multi-scale computational capability for the predictive understanding of the microstructure dynamics and its impact on thermal transport in nuclear fuel under irradiation with application to UO_2 as a model system.

Project Description: The goal of the *Center for Materials Science for Nuclear Fuel* is to develop a predictive multi-scale modeling framework that captures how defect generation and evolution and microstructure changes under irradiation lead to the degradation of fission-reactor fuel properties. Degradation of the thermo-mechanical behavior results from the cumulative, intricately coupled effects of fission-damage processes, high temperatures and high thermal gradients. Yet, apart from large empirical databases, a fundamental predictive science basis that connects "structure" across the relevant length and time scales with fuel behavior does not currently exist. To elucidate the underlying point-defect and microstructural mechanisms controlling this degradation behavior, we will develop a predictive computational framework based upon the non-linear dynamical theory of driven material systems and combining multi-scale models of defect and microstructure physics with complementary experimentation, on commensurate length scales. This unique combination of theory, computation and experiments will capture the complex interplay between the fission-induced defects and emerging microstructure with pre-existing grain structure, thus enabling the prediction of the impact of microstructure evolution on thermal transport in UO_2.

The Center brings together an internationally renowned, multi-institutional team of experimentalists and computational materials theorists focusing on understanding *microstructure science under irradiation*. The framework of non-linear dynamics of irradiation-driven materials will lead to an atomistically-informed generalized mesoscale phase-field model for the irradiation-induced microstructure evolution, which will furnish the defect state impacting thermal transport (see Fig. 1). This approach will capitalize on the team's demonstrated strength in theoretical and computational modeling of materials at all scales. In close synergy with the modeling effort, the experimental team will perform advanced microstructure, thermal-transport, and mechanical-property measurements on UO_2 using the unique experimental capabilities of DOE user facilities, including the Advanced Test Reactor (ATR), the Spallation Neutron Source (SNS) and the High Flux Isotopes Reactor (HFIR), and the Advanced Photon Source (APS), in addition to an array of state-of-the-art characterization techniques.

The availability of the new ATR National User Facility at INL not only gives the Center a distinct local dimension but also provides the unique capability of tying all of the experimental investigations to a true fission environment. Indeed, the ultimate goal of the Center is to develop an in-pile measurement capability to monitor degradation of critical components of the fuel assembly. This will enable us to develop new predictive models that can be benchmarked against actual ATR fuel data.

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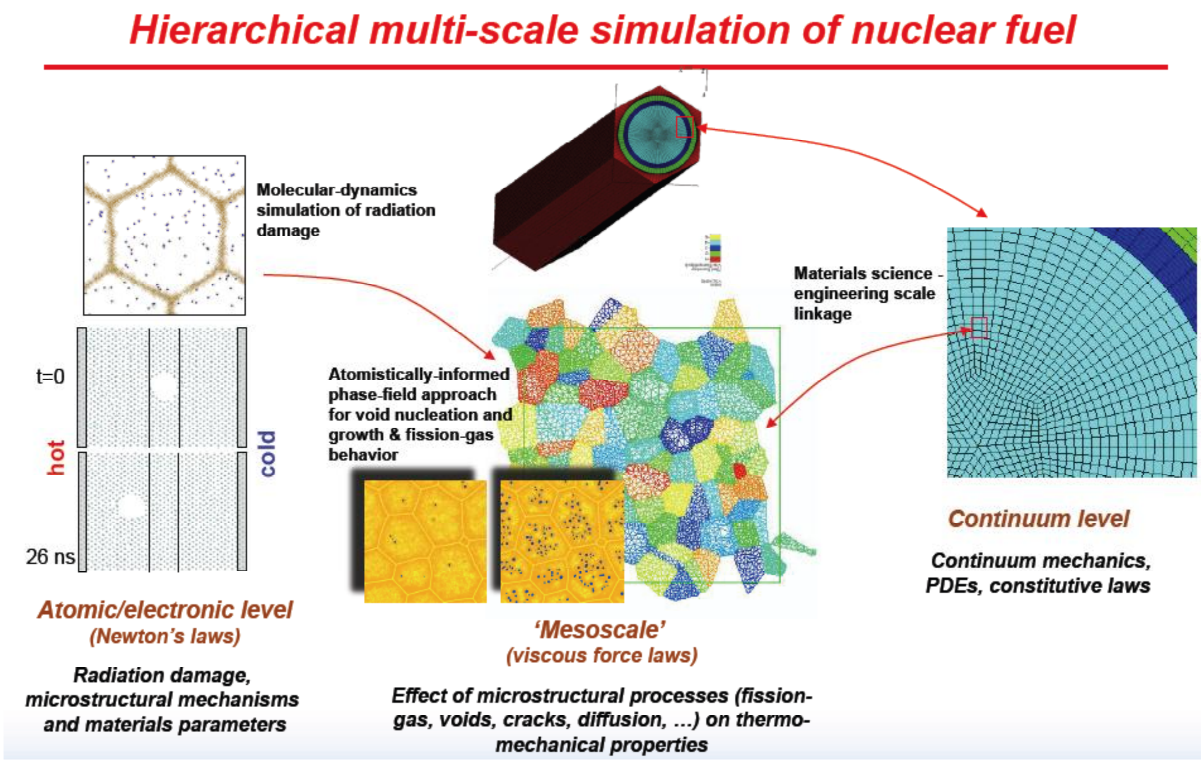

Fig. 1. The hierarchical multi-scale, multi-physics simulation approach developed through this EFRC combines three distinct levels:

- The ***atomic-level approach*** sketched on the left uses molecular-dynamics (MD) simulations in which the evolution of the system is followed based on the solution of Newton's equations of motion (typically over millions of time steps, or nanoseconds of real time).

- The quantified insights from the atomic-level simulations provide the input to the ***mesoscale approach*** based on a comprehensive phase-field model (center). The objects evolving in the mesoscale model are the microstructural elements such as the grain boundaries, dislocations, fission-gas bubbles, etc. The mesoscale elements evolve under the influence of thermodynamic forces. These ***atomistically-informed*** mesoscale simulations follow explicitly the evolution of the microstructure, typically over the order of milliseconds of real time.

- The output of the mesoscale simulations, "homogenized" in terms of net properties, such as the effective density, thermal conductivity and elastic moduli for a given state of temperature, stress and irradiation, serves as input into the ***continuum-level approach*** sketched on the right. The continuum calculations involve solution of a coupled set of partial differential equations, traditionally with materials input via empirical relations for the thermo-mechanical behavior of the material under the effects of irradiation. Here, via scale bridging down to the mesoscale, the continuum approach is ***microstructurally informed***.

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